

Determination of Am Fission Barriers from Calculated High-Dimensional Potential-Energy Surfaces

Peter Möller, T-16

In previous T-Division *Special Feature* and *Research Highlights* publications we have discussed calculations of fission potential-energy surfaces as functions of up to five different nuclear shape coordinates as the system evolves from a ground-state shape to two separated fission fragments. The five shape coordinates we consider beyond the second minimum in the fission barrier are elongation, neck radius, spheroidal deformations of the emerging left and right fragments, and left-right mass asymmetry. For less deformed shapes between the spherical shape and the second minimum in the barrier we consider three shape coordinates: ϵ_2 (quadrupole), ϵ_4 (hexadecapole), and γ (axial asymmetry). It is relatively straightforward (but a few thousand lines of fortran codes and scripts are required) by use of automated scripts to determine the height of the first, inner peak and of the second, outer peak in the fission barrier from the calculated potential-energy surfaces. We showed in the *Special Feature 2004* such results for a long chain of uranium isotopes. It is more complicated to develop completely automated scripts to determine additional features of the barriers. The reason is that it is not clear to what detail barriers need to be known for modeling fission cross sections and other quantities.

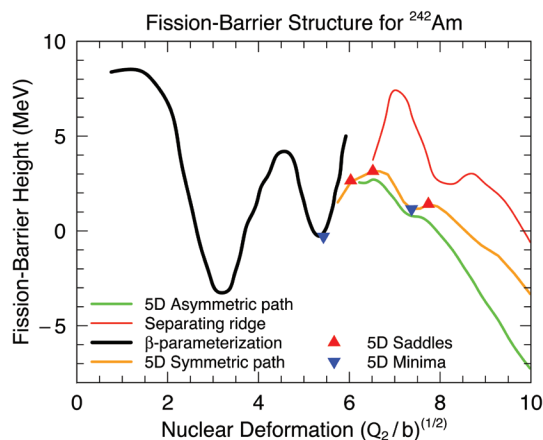
Actually, the detail needed would depend on the sophistication of the neutron-induced fission cross-section model. Currently many such models describe the fission barrier as a single-peaked parabolic barrier. However, it is anticipated that better accounting for the additional complexity of the fission barrier will result in cross-section models with better predictability. Such work is in progress.

As an example of our work on Am, we show in Fig. 1 some fission-barrier characteristics we have determined, by use of imaginary water-immersion techniques from the full potential-energy surfaces. The green curve in the right part of the figure represents a "valley," corresponding to mass-asymmetric shapes, in the potential energy surface. It is determined in the following way. For each Q_2 value considered in the calculation we locate all minima in the remaining 4-dimensional (4-D) space. Normally there are only 2 to 5 such minima that are deeper than a prescribed tolerance value.

For ^{242}Am we find that for each Q_2 value one of the minima always corresponds to a shape with emerging fragment masses around 140 and 100, which is the usual mean mass asymmetry observed in fission. Moreover, the shape of the large emerging fragment is near spherical, whereas the smaller fragment is well deformed. The green line connects the minima corresponding to this characteristic shape that we have identified for successive Q_2 values.

Another valley representing mass-symmetric shapes is also found and is shown in yellow. The red curve represents the ridge between these two valleys. In the full 5-D space we have furthermore located minima shown by downward-pointing blue triangles and saddles shown by upward-pointing red triangles. The thick black curve represents the potential energy from just beyond the sphere to slightly beyond the second minimum. It is obtained in the β multipole parameterization for successive β_2 values by minimizing the potential energy with respect to higher multipoles (up to β_6). We have earlier emphasized that such a procedure in general *does not* give potential energy curves that include the correct saddle points. In this case this deficiency is very visible: the right part of the thick black curve drastically overshoots the saddle points we have found in another parameterization in a full 5-D space. However, the minimum found in

Fig. 1. Structures identified in the calculated fission potential-energy for ^{242}Am .



this *different* shape parameterization at about $\sqrt{Q_2} = 5.5$ coincides very well with the second minimum on the black curve. This is a very important consistency check on our calculations. We have from other nonconstrained calculations verified that to the left of the second minimum the black curve properly represents the results that are obtained from full, higher-dimensional calculations.

Further analyses by water-flow techniques reveal that the saddle at $\sqrt{Q_2} = 6$ represents the saddle between the second minimum and the asymmetric (green curve) valley, whereas the saddle at $\sqrt{Q_2} = 6.5$ represents the saddle between the second minimum and the symmetric (yellow) valley. From the figure we see that a well-established asymmetric valley does not appear until slightly beyond the saddle corresponding to the asymmetric fission mode, whereas the symmetric valley is well manifested across the saddle corresponding to the symmetric fission mode. From Fig. 1 we obtain Fig. 2 in which the ^{242}Am barrier is represented as a *multiple-mode* fission barrier, in this case *bimodal*, asymmetric, and symmetric, in a form that might serve as a starting point for a more sophisticated model for (n,f) cross-section modeling than is a simple parabolic barrier. In this figure we also indicate a few representative nuclear shapes at various stages of the fission process.

In Fig. 3 we compare to experimental data for a sequence of Am isotopes calculated inner and outer barrier heights, which we have determined from an analysis similar to the one above for ^{242}Am . Especially the calculated outer barriers seem to show some systematic deviations from experimental data. However we need to observe that the barrier heights are not measured directly, they are deduced from modeling fission cross sections. Often these models assume a much simpler barrier structure than the one we have determined here and have phenomenological prescriptions for model features such as level densities. It is therefore desirable to model fission cross sections based on more realistic barriers such as the calculated ^{242}Am barrier shown in Figs. 1 and 2, and also to use calculated microscopic levels at the saddle points shown as starting points

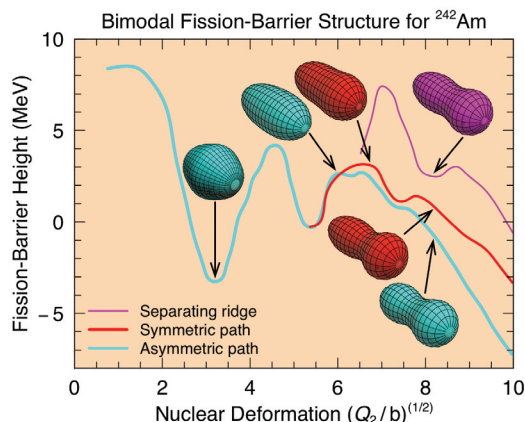


Fig. 2. Representation of the potential energy structure of ^{242}Am in terms of a bimodal fission barrier.

for level density modeling. Such work may lead to less phenomenological models and consequently more predictive models, and to better correspondence between calculated barriers and the “experimental” barriers that are extracted from fission-cross-section modeling.

For more information contact Peter Möller at moller@lanl.gov.

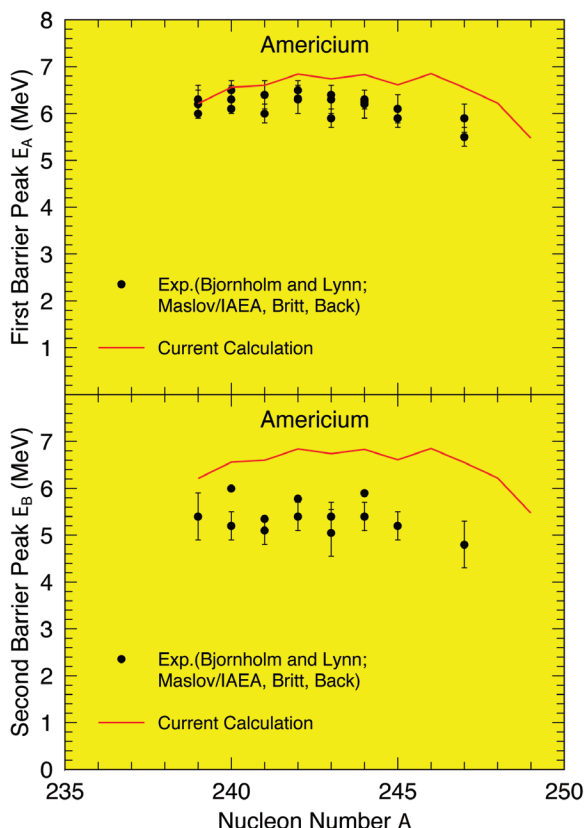


Fig. 2. Calculated inner and outer barrier heights for a sequence of Am isotopes compared to barrier heights deduced from experimental fission cross sections.